

# Quantum theory of heating of a single trapped ion

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The heating of trapped ions due to the interaction with a *quantized environment* is studied *without performing the Born-Markov approximation*. A generalized master equation local in time is derived and a novel theoretical approach to solve it analytically is proposed. Our master equation is in the Lindblad form with time dependent coefficients, thus allowing the simulation of the dynamics by means of the Monte Carlo Wave Function (MCWF) method.

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Single ions confined in miniaturized radio frequency traps can be cooled down by means of laser cooling techniques very efficiently [1]. Experiments have shown that the center of mass of a single cooled trapped ion undergoes a quantized harmonic oscillatory motion [2]. During the last decade a great deal of attention has been devoted to such systems since they turn out to be very weakly coupled to external environment, thus allowing the manipulation and observation of the coherent dynamics of a single quantum system [3]. Indeed, by irradiating the ion with properly configured laser beams, it is possible to manipulate the vibronic state of the ion. The easiness to engineer at will the interaction between the motional and internal degrees of freedom of the ion makes it possible to perform experimental tests of fundamental features of quantum mechanics. For example, many non-classical states of the oscillatory motion of the ion have been prepared and measured [4]. By using multiple ions in a linear Paul trap, experiments on quantum nonlocality have been performed [5] and many-particle entangled states have been realized [6]. Furthermore cold trapped ions have been recently proposed as a physical implementation for quantum computation [7].

Both for fundamental studies and for technological applications it is of great interest to understand and study those factors limiting the fidelity of the operations performed to manipulate coherently the quantum state of the ion. Heating of the center of mass oscillatory motion of one or more trapped ions seems to be one of the major practical sources of decoherence [8]. The process of heating of a single trapped ion is due to the electromagnetic coupling between noisy electric fields and the ion. Such fields give rise to fluctuating forces acting on the ion which can cause an increase in its motional energy. The physical origin of the noisy electric fields in the center of the trap has not yet been unambiguously identified. In fact, measurements of the heating rate are very difficult to perform since they require high sensitivity and they may depend on parameters related to the specific trap geometry used [8]. For this reason a general theory of heating would help in identifying and possibly reduce

the up to now unknown sources of noise.

Most of the theoretical studies on the heating of trapped ions deal with the interaction between a single harmonic oscillator and a reservoir which is either described as a classical stochastic field [9, 10, 11, 12] or as an infinite chain of quantum harmonic oscillators. In the first case an analytic solution for the dynamics of the system can be found without performing the Born-Markov approximation [9, 11]. In other words, it is possible to study the short time evolution of the heating function when the field noise spectrum is not flat, as it is indeed in any real experimental situation. However the analytical treatments, in this case, cannot describe the thermalization process, i.e. the long time behavior, since the stochastic field continuously feeds energy in the system, leading to an infinite growth of the heating function. On the other hand, modelling a thermal reservoir as an infinite chain of harmonic oscillators at temperature  $T$  allows, under certain approximations, to describe the dynamics of the system in terms of a master equation of the form [13]

$$\begin{aligned} \frac{\partial \hat{\rho}}{\partial t} = & - \Gamma(N+1) [\hat{a}^\dagger \hat{a} \hat{\rho} - 2\hat{a} \hat{\rho} \hat{a}^\dagger + \hat{\rho} \hat{a}^\dagger \hat{a}] \\ & - \Gamma N [\hat{a} \hat{a}^\dagger \hat{\rho} - 2\hat{a}^\dagger \hat{\rho} \hat{a} + \hat{\rho} \hat{a} \hat{a}^\dagger], \end{aligned} \quad (1)$$

where  $\hat{a}^\dagger$  and  $\hat{a}$  are the creation and annihilation operators of vibrational quanta,  $\Gamma$  is the heating constant and the environment is assumed to be at thermal equilibrium,  $N$  being the mean number of reservoir excitations at temperature  $T$ . In Eq. (1) the terms proportional to  $\Gamma(N+1)$  account for spontaneous and stimulated emission, that is a transfer of energy from the system to the reservoir, while the terms proportional to  $\Gamma N$  account for absorption, that is a transfer of energy from the reservoir to the system. The presence of the spontaneous emission term, arising from a quantized description of the reservoir, ensures the thermalization process. Indeed, from equation (1), it is possible to derive the following expression describing the time evolution of the heating function:

$$\langle \hat{n}(t) \rangle = n(\omega_0) (1 - e^{-\Gamma t}), \quad (2)$$

with  $n(\omega_0) = (e^{\beta \hbar \omega_0} - 1)^{-1}$ ,  $\beta = (KT)^{-1}$  and  $\omega_0$  frequency of the trap. In order to describe the dynamics of the system by means of the master equation (1), however, it is necessary to assume the validity of the Born-Markov approximation. As a consequence such a treatment is valid only for times  $t$  much bigger than the correlation time of the reservoir and thus does not give the correct short time behavior.

The aim of our paper is to study the heating of a single trapped ion interacting with a quantized reservoir *without performing the Born-Markov approximation*. One of the main results of the paper is the derivation of an analytical expression for the heating function describing both the non-Markovian short time behavior and the asymptotic thermalization process.

The Hamiltonian describing the interaction between the ion motion and a quantized reservoir modeled as an infinite chain of harmonic oscillators, can be written as follows  $\hat{H} = \hbar \sqrt{\alpha} \sum_{j=0}^{\infty} c_j (\hat{a} + \hat{a}^\dagger) (\hat{b}_j + \hat{b}_j^\dagger)$ , where  $\hat{b}_j$  is the annihilation operator of reservoir excitations and  $\alpha$  is the coupling strength. By using the time-convolutionless projection operator technique [14] and performing the Rotating Wave Approximation, we have derived the following master equation describing the non-Markovian dynamics of the system in the interaction picture:

$$\begin{aligned} \frac{\partial \hat{\rho}}{\partial t} = & - \frac{\bar{\Delta}(t) + \gamma(t)}{2} [\hat{a}^\dagger \hat{a} \hat{\rho} - 2 \hat{a} \hat{\rho} \hat{a}^\dagger + \hat{\rho} \hat{a}^\dagger \hat{a}] \\ & - \frac{\bar{\Delta}(t) - \gamma(t)}{2} [\hat{a} \hat{a}^\dagger \hat{\rho} - 2 \hat{a}^\dagger \hat{\rho} \hat{a} + \hat{\rho} \hat{a} \hat{a}^\dagger]. \end{aligned} \quad (3)$$

The functions  $\bar{\Delta}(t)$  and  $\gamma(t)$  are defined in terms of the two reservoir characteristic functions [15]: the correlation function  $\kappa(\tau) = \alpha \int_0^\infty \omega |g(\omega)|^2 (2n(\omega) + 1) \cos(\omega\tau) d\omega$  and the susceptibility  $\mu(\tau) = \alpha \int_0^\infty \omega |g(\omega)|^2 \sin(\omega\tau) d\omega$ , where  $n(\omega) = (e^{\beta \hbar \omega} - 1)^{-1}$ . Moreover, assuming a Lorentzian spectral density  $|g(\omega)|^2 = \omega_c^2 / [\pi(\omega^2 + \omega_c^2)]$  (Ohmic environment [16]) with  $\omega_c$  reservoir frequency cut, in the high temperature regime defined by the condition  $(\hbar\beta)^{-1} \gg \omega_c$  and in the weak coupling limit, the real functions  $\bar{\Delta}(t)$  and  $\gamma(t)$  can be written in a simple analytic form:

$$\begin{aligned} \bar{\Delta}(t) = & \frac{\alpha}{\hbar \beta \omega_0} \frac{r}{r^2 + 1} \left\{ e^{-\omega_c t} \sin(\omega_c t / r) \right. \\ & \left. + r [1 - e^{-\omega_c t} \cos(\omega_c t / r)] \right\}, \end{aligned} \quad (4)$$

$$\begin{aligned} \gamma(t) = & \frac{\alpha}{2} \frac{r^2}{r^2 + 1} \left[ 1 - e^{-\omega_c t} \cos(\omega_c t / r) \right. \\ & \left. - r e^{-\omega_c t} \sin(\omega_c t / r) \right], \end{aligned} \quad (5)$$

where  $r = \omega_c / \omega_0$ . Remembering that in the high temperature regime  $n(\omega_0) \simeq (\hbar \beta \omega_0)^{-1}$ , it is easy to check

that in the Markovian limit, that is when  $t \gg \tau_R$  with  $\tau_R = 1/\omega_c$  correlation time of the reservoir, equation (3) reduces to equation (1). The analytic expression of  $\bar{\Delta}(t)$  and  $\gamma(t)$  for a generic temperature  $T$  is, in general, more complicated. Nonetheless the temperature dependence of these coefficients of the master equation brings to light interesting features in the dynamics of the system and, for this reason, it is carefully discussed in a follow up paper [17].

Our non-Markovian master equation (3) has the general form of the time-convolutionless master equations [18, 19]. However, it is worth noting that it is not only local in time but also, as long as the coefficients  $\bar{\Delta}(t) + \gamma(t)$  and  $\bar{\Delta}(t) - \gamma(t)$  are positive, in the Lindblad form. We have verified that, for the value of parameters currently used in the experiments and for  $r > 1$  the time dependent sum and difference coefficients are positive at all times  $t$ . Note that the condition  $r > 1$  simply means that the spectral density of the reservoir overlaps with the frequency of oscillation of the ion, which is a reasonable and commonly done assumption. In other words, we demonstrate for the first time that the non-Markovian dynamics of the reduced density matrix of the system here considered, is described by a Lindblad-type master equation. Thus, it is possible to use the standard MCWF method to unravel Eq. (3) [20]. We note that up to now, only quantum state diffusion unravelings have been known and used for simulating the temporal behavior of a harmonic oscillator interacting with a non-Markovian quantized environment [21]. We would like to emphasize that the advantage of working with a master equation of Lindblad type whose analytical solution may be successfully found, as in our case, is that the positivity of the density matrix is ensured. In the following we will use the quantum jump MCWF method to obtain the temporal behavior of the heating function and compare it with the analytic solution.

We now briefly sketch the novel analytical treatment we have developed to solve the master equation (3) and derive a closed expression for the heating function describing both its short and its long time behavior. A detailed description of the method will be given elsewhere [17]. The first step of our approach consists in expanding the density matrix of the system as follows [22]:

$$\hat{\rho}(t) = \frac{1}{\pi} \int \chi_t(\lambda, \lambda^*) \exp(\lambda^* \hat{a} - \lambda \hat{a}^\dagger) d^2 \lambda \quad (6)$$

In Eq. (6),  $\lambda \in \mathbb{C}$  and  $\chi_t(\lambda, \lambda^*) = \text{Tr} \{ \exp(\lambda \hat{a}^\dagger - \lambda^* \hat{a}) \hat{\rho}(t) \}$  is the quantum characteristic function. Inserting Eq. (6) into Eq. (3) and by using some useful algebraic properties of the chronologically ordered time evolution superoperators  $\mathbf{T}_c(t)$  of the system, defined by  $\hat{\rho}(t) = \mathbf{T}_c(t) \hat{\rho}(0)$ , we obtain the following expression for the quantum characteristic

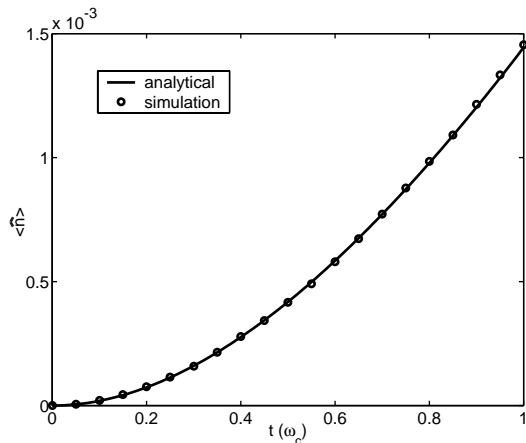


FIG. 1: Short time behavior of the heating function for coupling constant  $\alpha = 0.1Hz$ , trap frequency  $\omega_0 = 10^7 Hz$ ,  $r=10$  and  $T = 300K$ . We compare the analytic solution and the MCWF simulation with  $10^7$  histories.

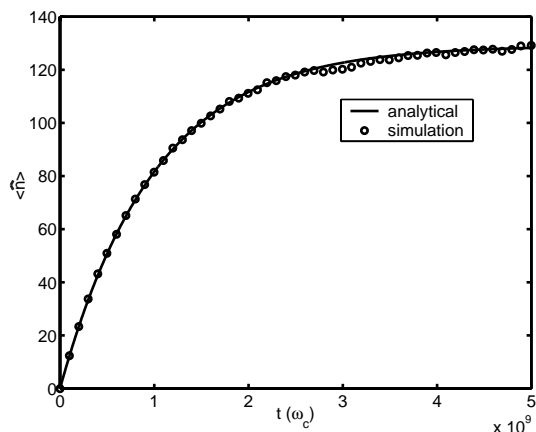


FIG. 2: Long time behavior of the heating function showing the thermalization process, for coupling constant  $\alpha = 0.1Hz$ , trap frequency  $\omega_0 = 10^7 Hz$ ,  $r=10$  and  $T = 10$  mK. We compare the analytic solution and the MCWF simulation with  $10^4$  histories. We note that, even for such a small value of the reservoir temperature, the high temperature approximation holds since  $(\hbar\beta)^{-1} \simeq 10^9 Hz$  which is one order of magnitude bigger than  $\omega_c$ .

function:

$$\chi_t(\lambda, \lambda^*) = \exp(-\Delta(t)|\lambda|^2) \chi_0 \left( T_\gamma^{1/2}(t)\lambda; T_\gamma^{1/2}(t)\lambda^* \right). \quad (7)$$

In this equation  $\chi_0$  is the quantum characteristic function at the initial time instant  $t = 0$ ,

$$T_\gamma(t) = \exp \left( -2 \int_0^t \gamma(t') dt' \right), \quad (8)$$

and

$$\Delta(t) = \int_0^t T_\gamma(t) T_\gamma^{-1}(t') \bar{\Delta}(t'). \quad (9)$$

The functions  $\bar{\Delta}(t)$  and  $\gamma(t)$  are defined by eqs. (4) and (5). For example, assuming as initial state a vibrational Fock state  $|k\rangle$ , Eq. (7) becomes

$$\chi_t(\lambda, \lambda^*) = \exp \left[ - \left( \Delta(t) + \frac{T_\gamma(t)}{2} \right) |\lambda|^2 \right] L_k(T_\gamma(t)|\lambda|^2), \quad (10)$$

where  $L_k(y)$  is the Laguerre polynomial of order  $k$  in  $y$ . Eq. (7) together with Eq. (6) gives the *analytic expression of the density matrix of the system in an operatorial form at any time instant  $t$* . From Eq. (7) it is easy to derive the following expression for the mean vibrational quantum number, i.e. for the heating function:

$$\langle \hat{n}(t) \rangle = \Delta(t) + \frac{1}{2} (T_\gamma(t) - 1) + k T_\gamma(t). \quad (11)$$

In Figs. 1 and 2 we show the short and long time behavior of the heating function of a trapped ion initially prepared in its vibrational ground state. We compare the analytical solution and the MCWF simulation performed starting from the master equation (3). The figures show a very good agreement between the analytical and the numerical approaches. We note that our quantum theory of heating predicts the initial quadratic behavior typical of non-Markovian dynamics. In Fig. 3 we compare the non-Markovian and Markovian time evolution for times  $t$  smaller than the reservoir correlation time  $\tau_R = 1/\omega_c$ . A similar result was deduced by James and by Budini in the case of a classical environment described in terms of a stochastic noisy electric field [9, 11]. Our approach, however, allows also to describe the asymptotic thermalization process as shown in Fig. 2. Indeed, for times  $t \gg \tau_R$  and for a flat reservoir spectrum  $r \gg 1$ , the heating function given by equation (11) reduces to the well known Markovian equation given by Eq. (2), as one can easily derive substituting the asymptotic expressions for  $\bar{\Delta}(t \rightarrow \infty)$  and  $\gamma(t \rightarrow \infty)$  into equations (8), (9) and (11), in the limit  $r \gg 1$ .

In conclusion we have proposed a new approach for studying the heating of a single trapped ion due to the interaction with a quantized reservoir. Our approach does not rely on the Born-Markov approximation and thus allows to describe the initial quadratic behavior of the heating function. Moreover, due to the quantum description of the environment, our solution describes correctly the thermalization process. Stated another way our quantum theory of heating bridges a gap existing in the literature. Until now, indeed, only non-Markovian analytical solutions, in the case of interaction with a classical environment, or Markovian analytical solutions, for interactions with a quantum environment, were known.

It is important to emphasize that measurements of the initial quadratic behavior of the heating function are difficult to perform for two reasons. Firstly because this would mean to make many measurements in an interval of time of the order of  $\tau_R \simeq 10^{-8}$  s, for the value of pa-

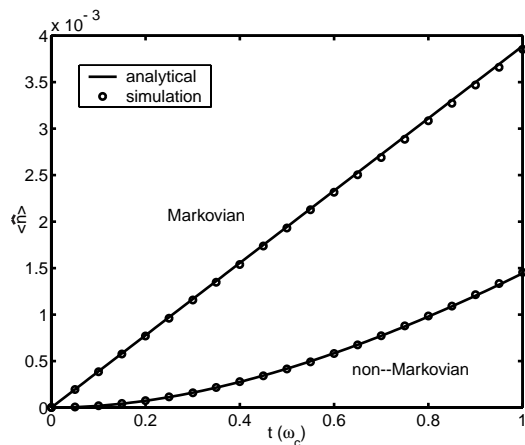


FIG. 3: Comparison between the short time Markovian and non-Markovian time evolutions of the heating function for coupling constant  $\alpha = 0.1 Hz$ , trap frequency  $\omega_0 = 10^7 Hz$ ,  $r=10$  and  $T = 300K$ .

rameters used in the paper. The second and more important reason is related to the difficulty in revealing so small variations in  $\langle \hat{n}(t) \rangle$  as the ones shown in Fig. 1. Very recently, however, it has been experimentally demonstrated the possibility of engineering both the type of reservoir interacting with a single trapped ion and the coupling between the system and the environment [23]. The analytical solution we have presented in this paper makes it possible to look for ranges of the relevant parameters of both the system and the reservoir in correspondence of which the non-Markovian quadratic behavior becomes experimentally observable.

The experimental ability in engineering reservoir suggests also another application. As we have already mentioned in the paper, we have analyzed the dependence of the coefficients of our master equation (3) on reservoir parameters such as its temperature  $T$  and frequency cut  $\omega_c$ . We have found that by changing such parameters the master equation passes from Lindblad type to non-Lindblad type. Such a modification does reflect a deep change in the dynamics of the system. This result will be discussed in more detail in a follow up paper since we believe that the possibility of studying analytically such changes may give more insight in understanding the fundamental properties of the heating process of single trapped ions.

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